Linear LS Parameter Estimation of Nonlinear Distribute Finite Element Models

E. Sparacino *,1, D. Madeo[1] and C. Mocenni[1]
[1]Dipartimento di Ingegneria dell'Informazione, Università di Siena.
*Via Roma, 56. 53100 Siena, Italy. Sparacino@dii.unisi.it

Abstract: This work concerns the development of a new direct parameter identification procedure for a class of nonlinear reaction-diffusion equations. We assume to know the model equations with the exception of a set of constant parameters, such as diffusivity or reaction term parameters. Using the Finite Element Method we are able to transform the original partial differential equation into a set of ordinary differential equations. A linear least squares (LS) method is then applied to estimate the unknown parameters by using normal equations. With this approach we reduce the effects of measurement errors and computational time compared with a nonlinear procedure.

Keywords: Reaction-diffusion equations, Parameter estimation, Inverse problems.

1 Introduction

Reaction-diffusion equations arise in many physical processes, such as physiological, ecological and social phenomena. Mathematical modelling of such systems often involves the estimation of the unknown parameters of the equations in order to reproduce as well as possible the dynamics of the real processes. However, the application of a parameter estimation process may involve nonlinear algorithms that make difficult the system identification procedures. Some effort in this direction has been done by the author in [6], where a simplified nonlinear two-step procedure is proposed and in [3], where, to the purpose of identification, a set of basis functions have been estimated.
The research reported herein concerns the development of a new parameter estimation procedure based on the finite element discretization of a class of nonlinear reaction-diffusion equations. In this context, a linear least square algorithm is applied to a reduced system consisting on a set of ordinary differential equations resulting from the time-space discretization (see [5] for the details on system identification).

The paper is organized as follows: Section 2 is focused on the description of the mathematical models used in the work. Section 3 describes the parameter estimation procedure. In Section 4 the use of Comsol Multiphysics in the context of the present work is explained. Section 5 presents the simulation results in terms of the fitting performance. We close in Section 6 with some final remarks and suggestions for further research.

2 The Model

We assume that the dynamic of the system is described by the following reaction-diffusion equation:

$$\frac{\partial u}{\partial t} - \nabla \cdot (\sigma \nabla u) = F(\theta, u) \quad \text{in } \Omega, \tag{1}$$

where σ is the diffusivity coefficient and $F(\theta,u) = \sum_m^{N_d} \theta_m u^m$. We suppose that $\Theta = [\sigma, \theta_1, \ldots, \theta_{N_d}]$ is an unknown vector to be estimated. Moreover, we assume that equation (1) is subject to suitable initial conditions and appropriate Neumann boundary conditions:

$$n \cdot (\sigma \nabla u) = 0 \quad \text{on } \partial\Omega, \tag{2}$$

where n is the outward normal vector.
Using finite element method, equation (1) can be transformed into a system of ordinary differential equations (see [4] for a detailed description of the finite element method).
The first step consists with multiplying each term by an arbitrary test function $w \in H^1(\Omega)$ to obtain the weak statement of the problem:

$$\left(\frac{\partial v}{\partial t}, w\right)_\Omega - \left(\nabla\left(\sigma \nabla v\right), w\right)_\Omega - (F, w)_\Omega = 0, \tag{3}$$

where $(\cdot,\cdot)_\Omega$ is the usual $L^2(\Omega)$ inner product:

$$(f,g)_\Omega = \int_\Omega f(x)g(x)d\Omega, \quad \forall f,g \in L^2(\Omega). \tag{4}$$

Applying the divergence theorem and using (2) we obtain:

$$\left(\frac{\partial v}{\partial t}, w\right)_\Omega + (\sigma\nabla v, \nabla w)_\Omega - (F,w)_\Omega = 0. \tag{5}$$

Let V_h be a finite dimensional subspace of $H^1(\Omega)$ spanned by the functions $\{\phi_{h1},\dots,\phi_{hN_p}\}$. Specifically, we consider $\phi_{hi}, i=1,\dots,N_p$ as a piecewise polynomials of degree 2 on a quasi uniform triangulation ρ_h of Ω with size h.
We look for a finite element approximation v_h to the solution v of the weak formulation (5) as a linear combination of the finite element basis functions $\phi_i(x)$ with time-dependent coefficients $U_i(t)$, namely:

$$v_h(t,x) = \sum_{i=1}^{N_p} U_i(t)\phi_i(x). \tag{6}$$

Substituting (6) into the weak form (5) and letting the test functions w run through the set of all basis functions $\{\phi_i\}_{i=1}^{N_p}$, we obtain the following finite element discretization of (1):

$$L(U) = A\dot{U} + \left(\sigma B - \sum_{m=1}^{N_d} \theta_m M_m(U)\right)U = 0, \tag{7}$$

where $U = \{U_i\}_{i=1}^{N_p}$ and

$$\begin{cases} A = (a_{i,j})_{i,j=1}^{N_p}, a_{i,j} = (\phi_i,\phi_j)_\Omega, \\ B = (b_{i,j})_{i,j=1}^{N_p}, b_{i,j} = (\nabla\phi_i,\nabla\phi_j)_\Omega, \\ M_m(U) = (\mu_{i,j}^m)_{i,j=1}^{N_p}, \\ \mu_{i,j}^m = \int_\Omega \phi_i \left(\sum_{k=1}^{N_d} U_k\phi_k\right)^{m-1} \phi_j d\Omega. \end{cases}$$

Equation (7) will be used for applying the parameter estimation procedure and to validate the identified model through numerical simulations.

3 Parameter Estimation

The parameter identification procedure is based on the minimization of a cost function, representing the mean square error between simulated and experimental data:

$$\widehat{\Theta} = \arg\min_\Theta J(\Theta, \widehat{U}, \bar{U}), \tag{8}$$

where $\bar{U}$ is the vector of real measurements that are assumed to be collected at each time instant in each nodal point of the finite element domain and $\widehat{U}$ is the vector of the model simulation.
Integrating equation (7) over a time interval $\Delta_t = [t_i, t_{i+1}]$, gives

$$\frac{U(t_{i+1}) - U(t_i)}{\Delta_t} = \tag{9}$$
$$= A^{-1}\int_{t_i}^{t_{i+1}} \left(-\sigma B + \sum_{i=1}^{N_d} \theta_i M_i(U(t_i))\right) U(t_i)d\tau.$$

Considering Equation (9) for $i = 1,\dots,T-1$, we obtain a linear system of equations in the variable $\Theta := (\sigma, \theta_1,\dots,\theta_{N_d})'$ of the form

$$Y \;=\; W\;\Theta, \tag{10}$$

where

$$Y = \left(\frac{U(t_{i+1}) - U(t_i)}{\Delta_t}\right)_{i=1,\dots T-1} \tag{11}$$

and

$$\begin{aligned} W = \Big(&-A^{-1}B\textstyle\int_{t_i}^{t_{i+1}} U, \\ &\textstyle\int_{t_i}^{t_{i+1}} A^{-1}M_1(U(t_i))U(t_i)d\tau,\dots, \\ &\textstyle\int_{t_i}^{t_{i+1}} A^{-1}M_{N_d}(U(t_i))U(t_i)d\tau\Big)_{i=1,\dots T-1}. \end{aligned} \tag{12}$$

If we replace U by the measurements $\bar{U}$, and approximate the integrals in (9) by numerical quadrature, equation (10) becomes

$$Y \;=\; \widetilde{W}\;\Theta \;+\; e, \tag{13}$$

where e is an error caused by noise and numerical quadrature, and $\widetilde{W}$ is the approximate value of W.
We can now compute a least squares estimate of Θ in (13) as:

$$\Theta_{LS} = (\widetilde{W}'\;\widetilde{W})^{-1}\;\widetilde{W}'Y. \tag{14}$$

This method can be easily implemented in Comsol Multiphysics as shown in the next Section.

4 Use of COMSOL Multiphysics

The Comsol Multiphysics linearization of the finite element model (7), used in the Newton iteration, is:

$$D(\dot{U} - \dot{U}_0) + K(U - U_0) = L(U_0), \quad (15)$$

where $D = -\partial L/\partial \dot{U}$ and $K = -\partial L/\partial U$ are the mass and the stiffness matrices, respectively (see the Comsol Multiphysics user's guide [2] for a detailed description).
Computing these matrices for system (7) leads to:

$$\begin{array}{l} D = -\partial L/\partial \dot{U} = -A, \\ K = -\partial L/\partial U = -\sigma B + \sum_{m=1}^{N_d} \theta_m m M_m(U). \end{array} \quad (16)$$

Note that, for different values of $\Theta := (\sigma, \theta_1, \ldots, \theta_{N_d})'$, we are able to obtain different matrices Ks. In particular, we have:

$$\begin{cases} K = B, & \text{for} \quad \Theta = (-1, 0, \ldots, 0)' \\ K = M_m(U), & \text{for} \quad \Theta(m+1) = \frac{1}{m}, \end{cases} \quad (17)$$

with $m = 1, \ldots, N_d$.
This fact allows us to easily compute matrix W in (12) by the Comsol Multiphysics command *assemble* [1].
Here is reported a piece of Comsol pseudocode:

```
fem.Theta(1)=-1;
[A,B] = assemble(fem,'Out',{'D' 'K'})

for t = 1 : T
for m = 1 : Nd
fem.Theta = 0;
fem.Theta(m+1) = 1/m;
Mm(m) = assemble(fem,'Out',{'K'},'U',UM(t));
end
end
```

where UM(t) is the vector of real measurements at time t.
The model parameters can now be easily computed by equation (3).

5 Simulation Results

In order to numerically validate the results, we apply the method to a nonlinear model describing the distribution of a population in a square domain. The spatio-temporal dynamics is described by the following equation with a nonlinear logistic equation:

$$\frac{\partial u}{\partial t} - \nabla \cdot (\sigma \nabla u) = ru\left(1 - \frac{u}{k}\right) \quad \text{in } \Omega. \quad (18)$$

For the parameter identification problem, we set $\Theta = (\sigma, r, r/k)$ and compute the finite element model as in Sections 2 and 3.
The vector of real measurements $\bar{U}$ is obtained by simulating the model in a domain $\Omega = (10 \times 10)$ with the following parameter values:

Par.	Value
σ	1e-2
r	1e-1
k	10

Table 1: Nominal parmeter values.

and a mesh consisting of 841 nodal points.
We test the parameter estimation procedure by using equation (18) with different initial conditions and mesh dimension. In particular, we use meshes consisting of and 81, 121 and 256 nodal points and the following initial conditions:

$$u(x, y, 0) = x \quad (19a)$$

$$u(x, y, 0) = sin\left(\frac{\pi}{2}x\right) + a, \quad (19b)$$

where a is a positive parameter introduced to avoid negative values in the initial state. The fitting performance is evalueted in terms of the spatial mean square error between measurements $\bar{U}$ and simulated data $\widehat{U}$:

$$\text{MSE(t)} = \frac{1}{N_p} \sum_{i=1}^{N_p} \left(\frac{\bar{U}(i,t) - \widehat{U}(\Theta_{LS}, i, t)}{\bar{U}(i,t)} \right)^2. \quad (20)$$

Figures 1 and 2 report the obtained MSEs for the considered cases.
As we can see, the model performs better using a finer mesh. However, the error remain low also for coarser meshes. Tables 2 and 3 report the values of the estimated parameters for different N_p and initial conditions (19a) and (19b), respectively.

Par.	$N_p = 81$	$N_p = 121$	$N_p = 256$
σ	1.055e-2	0.998e-2	0.967e-2
r	0.983e-1	0.989e-1	0.995e-1
k	9.999	9.999	9.998

Table 2: Estimated parameter values for initial condition (19a).

Par.	$N_p = 81$	$N_p = 121$	$N_p = 256$
σ	0.875e-2	0.934e-2	0.986e-2
r	0.999e-1	0.995e-1	0.999e-1
k	9.990	9.996	9.996

Table 3: Estimated parameter values for initial condition (19b) .

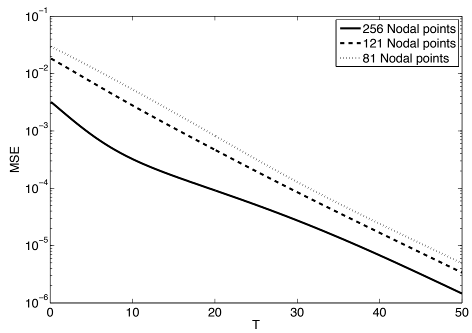

Figure 1: MSE between simulated and real measurements data for different values of N_p and initial condition (19a).

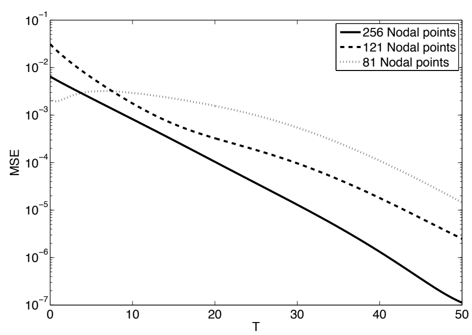

Figure 2: MSE between simulated and real measurements data for different values of N_p and initial condition (19b).

6 Conclusion

This paper addresses the problem of estimating the parameter of a class of nonlinear reaction-diffusion equations. After a finite element discretization of the model, a linear least square method is applied to the resultant system of ordinary differential equations in order to retrieve the parameter values. The identification procedures are performed by considering two different initial conditions and three mesh dimensions.

The use of Comsol Multiphysics command *assemble* plays a crucial role in finding the fem matrices.

Finally, the fitting performances of the estimated models are presented and evaluated in terms of the spatial mean square error.

Future work will concern parameter sensitivity analysis with respect to different initial conditions and mesh dimension. Furthermore, a comparison with nonlinear methods will be considered.

References

[1] Comsol, *Comsol Multiphysics Reference Guide, v.3.5a*, Comsol AB, 2008.

[2] ———, *Comsol Multiphysics User's Guide, v.3.5a*, Comsol AB, 2008.

[3] L. Guo and SA Billings, *Identification of Partial Differential Equation Models for Continuous Spatio-Temporal Dynamical Systems*, IEEE Transactions on Circuits and Systems II: Express Briefs **53** (2006), no. 8, 657–661.

[4] T.J.R. Hughes, *The finite element method: linear static and dynamic finite element analysis*, Prentice-Hall Englewood Cliffs, NJ, 1987.

[5] L. Ljung, *System identification*, Springer, 1987.

[6] C. Mocenni and E. Sparacino, *Identification and simulation of a spatial ecological model in a lake with fractal boundary*, Mathematics and Computers in Simulation **79** (2009), 3534–3546.